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Abstract

A macroscopic system modelling the chemotactic motion of bacteria is considered. This model has been obtained in a previous work thanks to a hydrodynamical limit of a kinetic system. Existence and uniqueness of measure solutions for this system using the concept of duality solution have been proved by the authors in [7]. In this paper, we investigate the numerical discretization of this system. A scheme based on a finite volume approach is proposed and the convergence of the numerical solution towards the unique duality solution is stated. Numerical simulations are provided that shows the behaviour of solutions after blow up.

Keywords: chemotaxis, non-local conservation equations, numerical analysis, finite volume scheme, measure-valued solutions

2010 AMS subject classifications: Primary: 35Q92, 35L60, 65M08; Secondary: 35D30

1 Introduction

Chemotaxis is the phenomenom in which a population of cells rearranges its structure according to the behaviour of some chemical present in the environment. In this work, we focus on the following macroscopic model for chemotaxis:

$$\partial_t \rho + \partial_x (a(\partial_x S)\rho) = 0, \tag{1}$$

$$a(\partial_x S) = -c\,\phi(c\partial_x S), \tag{2}$$

$$-\partial_{xx} S + S = \rho. \tag{3}$$

In this system, $\rho(t,x) \geq 0$ denotes the density of cells at time $t \geq 0$ and position $x \in \mathbb{R}$, and $S(t,x)$ is the concentration of the chemical, which is here produced by the bacteria at a rate proportional to their density, and diffuses in the system. The positive constant c corresponds to the individual velocity of cells, whereas a is a macroscopic velocity. The real-valued function ϕ describes the influence of the chemoattractant concentration S on the global motion of bacteria. When ϕ is nonincreasing, hence a nondecreasing, cells attract themselves, we are in the case of *positive chemotaxis*, the chemical is then called the *chemoattractant*, otherwise, we are in the repulsive case and speak about the *chemorepellant*. We complement this system with the boundary conditions

$$\rho(t=0,x) = \rho^{ini}(x), \qquad \lim_{x\to\pm\infty} \rho(t,x) = 0, \qquad \lim_{x\to\pm\infty} S(t,x) = 0. \tag{4}$$

Introducing the elementary interaction kernel K solving $-\partial_{xx}K + K = \delta_0$, i.e. $K = \frac{1}{2}e^{-|x|}$, the latter system reduces to the nonlocal scalar conservation law

$$\partial_t \rho + \partial_x(a(\partial_x K * \rho)\rho) = 0. \tag{5}$$

When a is nondecreasing, this equation is known as the aggregation equation. It is now classical that regular solutions blow up in finite time when K is not smooth (see e.g. [1]). Thus measure solutions have to be considered, together with a suitable definition of the product $a(\partial_x K * \rho)\rho$, when ρ is a measure.

System (1)–(3) can be obtained thanks to a hydrodynamical limit of the so-called Othmer-Dunbar-Alt model. This system has been introduced to take care of the *run and tumble* process: the motion of cells is due to the alternance of a swim phase in a given direction (*run*) and of a reorientation phase during which cells take a new direction for the next run (*tumble*). Denoting $f(t, x, v)$ the distribution function at time t, position $x \in \mathbb{R}$ and velocity $v \in \{-c, c\}$, the kinetic system of equations writes in one space dimension (see e.g. [5])

$$\partial_t f_\varepsilon + v\partial_x f_\varepsilon = \frac{1}{\varepsilon}((1 + \phi(-v\partial_x S_\varepsilon))f_\varepsilon(-v) - (1 + \phi(v\partial_x S_\varepsilon))f_\varepsilon(v)), \tag{6}$$

$$-\partial_{xx} S_\varepsilon + S_\varepsilon = \rho_\varepsilon = f_\varepsilon(v) + f_\varepsilon(-v). \tag{7}$$

The real c represents the constant velocity of cells. The left-hand side describes the run phase whereas the right-hand side models the tumble phase. The operator $T[S] := \frac{1}{2}(1 + \phi(-v\partial_x S))$ is called the turning rate and corresponds to the rate of reorientation of cells. Obvioulsy we should have $0 \leq T[S] \leq 1$. The parameter ε is a scaling factor which is assumed here to be very small ($\varepsilon \ll 1$). This corresponds to the phenomenon of domminant taxis. Other scalings are possible, that lead eventually to drift-diffusion equations such as the classical Keller-Segel model.

The hydrodynamic limit consists in letting $\varepsilon \to 0$, and it is easily checked that formally the solution $(\rho_\varepsilon, S_\varepsilon)$ of the kinetic system converges to some solution (ρ, S) of system (1)–(3). A complete proof of this result is given in [7], together with a global-in-time existence and uniqueness of duality solutions for system (1)-(3). The main drawback of this method is that, since duality solutions are presently defined only in one space dimension, we are limited to $x \in \mathbb{R}$. On the other hand, existence of measure-valued solutions for the aggregation equation (5) has been obtained in [4] in any space dimension. The authors make use of optimal transport technique: in this geometric approach, the solution appears as a gradient flow for the interaction energy. However, this latter tool is not so convenient to build numerical schemes and to obtain numerical simulations.

The aim of this paper is therefore to propose a numerical scheme based on a finite volume approach to get numerical simulations of solutions to the macroscopic model (1)–(3). The main ingredient is a proper definition of the flux $J = a(\partial_x S)\rho$. The outline is the following. In the next Section we recall some definitions and the existence result stated in [7]. In Section 3 we present the scheme and state some of its main properties in the attractive case. Finally Section 4 provides numerical simulations, both in the attractive and the repulsive case.

2 Existence of duality solutions

Let us denote by $\mathbf{M}_b(\mathbb{R})$ the set of bounded Radon measures and by $\mathbf{P}_1(\mathbb{R})$ the set of nonnegative measures in $\mathbf{M}_b(\mathbb{R})$ with finite first moment, that is $\int_{\mathbb{R}} |x| d\mu(x) < \infty$. Duality solutions have been introduced in [2] to solve scalar conservation laws with discontinuous coefficients. More precisely, it gives sense to measure valued solutions of the scalar conservation law

$$\partial_t \rho(t, x) + \partial_x(b(t, x)\rho(t, x)) = 0,$$

where $b \in L^\infty((0,T)\times\mathbb{R})$ satisfies the so-called one-sided Lipschitz (OSL) condition

$$\partial_x b(t,.) \le \beta(t) \qquad \text{for } \beta \in L^1(0,T), \text{ in the distributional sense.} \tag{8}$$

We refer to [2] for the precise definition and general properties of these solutions. In this framework we define duality solutions of the studied system in the spirit of [3]:

Definition 2.1 *We say that $(\rho, S) \in C([0,T];\mathbf{M}_b(\mathbb{R})) \times C([0,T];W^{1,\infty}(\mathbb{R}))$ is a duality solution to (1)–(3) if there exists $a \in L^\infty((0,T)\times\mathbb{R})$ and $\alpha \in L^1_{loc}(0,T)$ satisfying $\partial_x a \le \alpha$ in $\mathbf{D}'(\mathbb{R})$, such that*

(i) for all $0 < t_1 < t_2 < T$

$$\partial_t \rho + \partial_x(a\rho) = 0 \quad \text{in the sense of duality on }]t_1, t_2[,$$

(ii) equation (2) is satisfied in the weak sense :

$$\forall\, \psi \in C^1(\mathbb{R}),\ \forall\, t \in [0,T], \quad \int_{\mathbb{R}} (\partial_x S \partial_x \psi + S\psi)(t,x)\, dx = \int \psi(x)\, \rho(t, dx),$$

(iii)

$$a = a(\partial_x S) \quad a.e.$$

The OSL estimate suggests that the velocity field a has to be compressive, that is to satisfy the OSL estimate. Therefore we assume to be in the case of positive chemotaxis. Then cells attract themselves and a is non-decreasing; more precisely we assume

$$a \in C^1(\mathbb{R}), \qquad 0 \le a' \in L^\infty(\mathbb{R}), \qquad \forall\, x \in \mathbb{R} \quad |a(x)| \le c. \tag{9}$$

The latter estimate means that the collective displacement of cells should not be faster than the velocity of each individual cell; it is a direct consequence of the fact that the turning rate $T[S]$ satisfies $0 \le T[S] \le 1$.

Moreover we have a natural one-sided estimate on the potential S when ρ is nonnegative. In fact, from (3) $\partial_{xx} S \le S$. This estimate can be considered as an entropy estimate for the scalar conservation law (1) which is crucial for the proof of uniqueness of solutions (see Theorem 5.1 of [7]). From now on, we will define by A the antiderivative of a which vanishes at 0. We have from the chain rule that, when it is defined, the product

$$a(\partial_x S)\rho = a(\partial_x S)(-\partial_{xx} S + S) = -\partial_x(A(\partial_x S)) + a(\partial_x S)S.$$

Then a natural definition of the flux is given by

$$J = -\partial_x(A(\partial_x S)) + a(\partial_x S)S. \tag{10}$$

We are now in position to state the existence and uniqueness result of [7].

Theorem 2.2 *Let us assume that ρ^{ini} is given in $\mathbf{P}_1(\mathbb{R})$ and that (9) is satisfied. Then, for all $T > 0$ there exists a unique duality solution (ρ, S) with $0 \le \rho \in \mathbf{P}_1(\mathbb{R})$ of (1)–(3) which satisfies in the distributional sense :*

$$\partial_t \rho + \partial_x J = 0, \tag{11}$$

where J is the flux defined in (10). Moreover, there exists a universal representative, denoted $\widehat{a}$, such that $\widehat{a} = a(\partial_x S)$ a.e. and

$$\widehat{a}\rho = J, \quad \text{in the sense of measures.}$$

Then, we have $\rho = X_\# \rho^{ini}$ where X is the backward flow corresponding to $a(\partial_x S)$.

Remark 1 *This theorem is proved in [7] with a weaker assumption than (9). However, this stronger assumption is needed here for the numerical analysis.*

3 Numerical scheme

3.1 Discretization

Let us consider a uniform space discretization with step δx and denote by δt the time step, and set $\lambda = \delta t/\delta x$. Then $t_n = n\delta t$ and $x_i = x_0 + i\delta x$. We assume that $(\rho_i^n)_{0\le i\le N}$ is an approximation of $(\rho(t_n, x_i))_{0\le i\le N}$. We obtain an approximation ρ_i^{n+1} of $\rho(t_{n+1}, x_i)$ by using the following Lax-Friedrichs discretization of equations (11)–(10):

$$\rho_i^{n+1} = \rho_i^n(1-\lambda c) + \frac{\lambda}{2}c(\rho_{i-1}^n + \rho_{i+1}^n) + \frac{\lambda}{2}(J_{i-1/2}^n - J_{i+1/2}^n), \tag{12}$$

$$J_{i+1/2}^n = -\frac{A(\partial_x S_{i+1}^n) - A(\partial_x S_i^n)}{\delta x} + a_{i+1/2}^n \frac{S_{i+1}^n + S_i^n}{2}. \tag{13}$$

We recall that c denotes the constant modulus of the velocity of cells, and the velocity $a(\partial_x S)$ is discretized as

$$a_{i+1/2}^n = \begin{cases} 0 & \text{if } \partial_x S_{i+1}^n = \partial_x S_i^n, \\ \dfrac{A(\partial_x S_{i+1}^n) - A(\partial_x S_i^n)}{\partial_x S_{i+1}^n - \partial_x S_i^n} & \text{otherwise,} \end{cases} \tag{14}$$

complemented with the standard centered finite difference $\partial_x S_{i+1}^n = \dfrac{S_{i+2}^n - S_i^n}{2\delta x}$. We couple this equation with the following standard discretization of the equation for the chemoattractant (3)

$$-\frac{S_{i+1}^n - 2S_i^n + S_{i-1}^n}{\delta x^2} + S_i^n = \rho_i^n. \tag{15}$$

In order to avoid the treatment of boundary conditions, we assume that the solutions are compactly supported in the computational domain. Then from now on, we have that $\rho_0^n = S_0^n = S_1^n = J_{-1/2}^n = 0$ and $\rho_N^n = S_N^n = J_{N+1/2}^n = 0$.

3.2 Numerical analysis

Before stating and proving our convergence result, we start by a Lemma which proves a CFL-like condition for the scheme :

Lemma 3.1 *Let us assume that (9) holds and that the condition*

$$\lambda := \frac{\delta t}{\delta x} \le \frac{2}{3c}, \tag{16}$$

is satisfied. Then the scheme defined in (12)–(15) is nonnegative.

Proof. Let us assume that $\rho_i^n \ge 0$. From (14)–(15) we deduce that we can rewrite (13) as

$$J_{i+1/2}^n = a_{i+1/2}^n \frac{\rho_{i+1}^n + \rho_i^n}{2}. \tag{17}$$

Thus we can rewrite (12)

$$\rho_i^{n+1} = \rho_i^n\left(1 - \lambda c + \frac{\lambda}{4}(a_{i-1/2}^n - a_{i+1/2}^n)\right) + \frac{\lambda}{2}\left(c + \frac{a_{i-1/2}^n}{2}\right)\rho_{i-1}^n + \frac{\lambda}{2}\left(c - \frac{a_{i+1/2}^n}{2}\right)\rho_{i+1}^n. \tag{18}$$

Moreover, by assumption (9) we have $|a_{i+1/2}^n| \le c$ for all $i = 0, \dots, N$. Therefore, if $\lambda \le \frac{2}{3c}$, all the coefficients in front of ρ_{i-1}^n, ρ_i^n and ρ_{i+1}^n are nonnegative. We conclude that the scheme is nonnegative. □

Let us define

$$\rho_\delta(t,x) = \sum_{n\in\mathbb{N}} \sum_{i=0}^{N} \rho_i^n \mathbf{1}_{[n\delta t,(n+1)\delta t)\times[x_i,x_{i+1})}(t,x),$$

and S_δ, $\partial_x S_\delta$, J_δ and a_δ are defined in a similar way thanks to $(S_i^n)_i$, $(\partial_x S_i^n)_i$, $(J_{i+1/2}^n)_i$ and $(a_{i+1/2}^n)_i$.

Theorem 3.2 *Let us assume that we are given $\rho^{ini} \in \mathbf{P}_1(\mathbb{R})$ and define $\rho_i^0 = \int_{x_i}^{x_{i+1}} \rho^{ini}(dx) \geq 0$. Under assumption (9), if (16) is satisfied, then the discretization (ρ_δ, S_δ) converges towards the solution (ρ, S) of Theorem 2.2 as δt and δx go to 0.*

Proof. We first notice that since the matrix of the linear system (15) is a $M-$matrix, we have that if $(\rho_i^n)_i$ is nonnegative, then $S_i^n \geq 0$ for all $i = 0, \dots, N$.

Let us define $M_i^n = \delta x \sum_{j=0}^{i} \rho_j^n$ and $M_i^{n+1} = \delta x \sum_{j=0}^{i} \rho_j^{n+1}$. Since the scheme (12) is conservative, we have $M_N^n = M_N^0$. Clearly, $\rho_i^n = (M_i^n - M_{i-1}^n)/\delta x$ and from (17) we have $J_{i+1/2}^n = a_{i+1/2}^n (M_{i+1}^n - M_{i-1}^n)/(2\delta x)$. Then we deduce from (12) that

$$M_i^{n+1} = (1-\lambda c) M_i^n + \frac{\lambda}{2}\left(c - \frac{a_{i+1/2}^n}{2}\right) M_{i-1}^n + \frac{\lambda}{2}\left(c + \frac{a_{i+1/2}^n}{2}\right) M_{i+1}^n. \tag{19}$$

If λ satisfies (16), we have $\lambda c < 1$ moreover, by assumption (9), $|a_{i+1/2}^n| \leq c$. Thus M_i^{n+1} is a convex combination of M_{i-1}^n, M_i^n and M_{i+1}^n. We deduce that provided condition (16) is satisfied, we have $0 \leq \rho_i^n = (M_i^n - M_{i-1}^n)/\delta x$ and equation (18) implies a $BV(\mathbb{R})$ estimate on $(M_i^n)_i$. Moreover, for all $i = 0, \dots, N$, we have $M_i^n \leq M_N^n = M_N^0$ which provides a L^∞ estimate on $(M_i^n)_i$.

Summing (15), we get

$$M_i^n = \delta x \sum_{j=0}^{i} S_j^n - 2\partial_x S_i^n. \tag{20}$$

We deduce that $0 \leq \delta x \sum_{j=0}^{N} S_j^n \leq M_N^n$. Then we have a $L^\infty \cap BV(\mathbb{R})$ estimate on $(\partial_x S_i^n)_i$.

Let us define

$$M_\delta(t,x) = \sum_{n\in\mathbb{N}} \sum_{i=0}^{N} M_i^n \mathbf{1}_{[n\delta t,(n+1)\delta t)\times[x_i,x_{i+1})}(t,x).$$

Using standard arguments, we have a $L^\infty \cap BV((0,T)\times\mathbb{R})$ estimate on M_δ. It implies the convergence, up to a subsequence, of M_δ in $L^1_{loc}(\mathbb{R}^+\times\mathbb{R})$ towards a function $M \in L^\infty \cap BV((0,T)\times\mathbb{R})$ when δt and δx go to 0 and satisfy (16). By the same token we have the strong convergence in $L^1_{loc}(\mathbb{R}^+\times\mathbb{R})$ of $\partial_x S_\delta$ towards $\partial_x S$ and by definition of $\partial_x S_i$ we have the convergence in $L^1_{loc}(\mathbb{R}^+, W^{1,1}_{loc}(\mathbb{R}))$ of S_δ towards S. Let us define, in the weak sense, $\rho = \partial_x M \in \mathbf{M}_b(\mathbb{R})$. Obviously, noting that $\rho_i^n = (M_i^n - M_{i-1}^n)/\delta x$, we deduce that ρ is the limit in the distributional sense of ρ_δ. Passing to the limit in the equation (20) we deduce that S is a weak solution of equation (3).

Moreover we have

$$\frac{A(\partial_x S_{i+1}^n) - A(\partial_x S_i^n)}{\partial_x S_{i+1}^n - \partial_x S_i^n} = a(\theta_i^n), \qquad \theta_i^n \in (\partial_x S_i^n, \partial_x S_{i+1}^n).$$

Using assumption (9), we deduce that the sequence $(a_\delta)_\delta$ is bounded in L^∞, thus we can extract a subsequence converging in $L^\infty - weak^*$ towards $\widetilde{a}$. From the L^1_{loc} convergence of $(\partial_x S_\delta)_\delta$, we deduce that $\widetilde{a} = a(\partial_x S)$ a.e. Then, from (13), we have the convergence in the sense of distributions of J_δ towards $J = -\partial_x(A(\partial_x S)) + a(\partial_x S)S$ a.e. Finally, taking the limit in the distributional sense of equation (12) we deduce that ρ is a distributional solution to (11)–(10). By uniqueness of this solution, we deduce that (ρ, S) is the unique duality solution of Theorem 2.2. □

4 Numerical simulations

We present in this section some numerical results obtained thanks to an implementation of the scheme (12)–(15). Even though the scheme was designed to ensure convergence in the attractive case, we evidence that it gives interesting results in the repulsive case as well.

In all the following, the computational domain is assumed to be $[-2.5, 2.5]$ and the velocity c is normalized to 1.

4.1 Attractive case

Let us consider the function $a(x) = 2/\pi$ Arctan$(10x)$, which satisfies clearly (9). In Figure 1, we plot the dynamics for the smooth initial data:

$$\rho^{ini}(x) = e^{-10(x-1.25)^2} + 0.8e^{-20x^2} + e^{-10(x+1)^2}.$$

We notice that the blow-up occurs fastly. Then after a small time, solutions are formed by 3 peaks which can be considered as numerical Dirac masses. Then the Dirac masses move and collapse in finite time. This behaviour is very similar to the one observed in [7] where a particle method has been implemented.

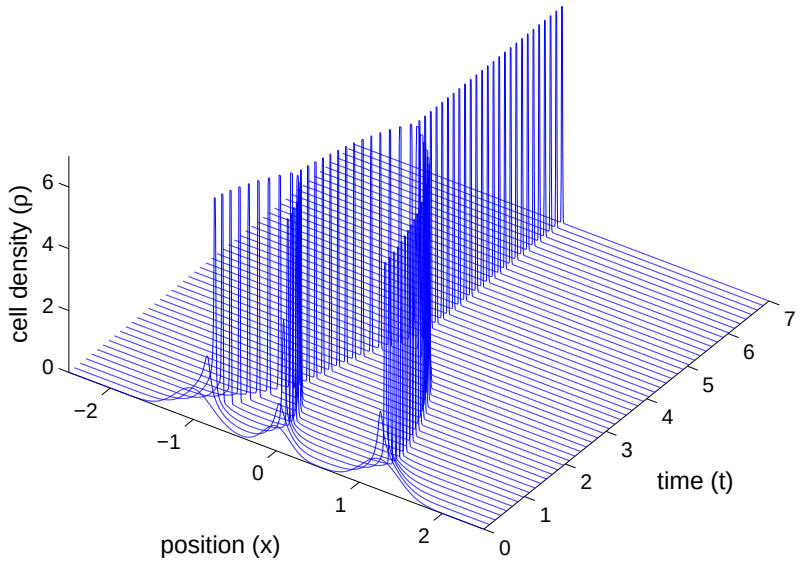

Figure 1: Dynamics of the cell density for an initial data given by a sum of 3 regular bumps. We notice the fast blow up of solutions, then the obtained aggregates collapse together.

4.2 Repulsive case

It is very interesting to see the numerical results obtained by this scheme in the repulsive case, i.e. when the function a is non-increasing. In Figure 2, we present the result for $a(x) = -2/\pi$ Arctan$(10x)$ (left) and $a(x) = -2/\pi$ Arctan$(50x)$. The initial data is $\rho^{ini}(x) = e^{-10x^2}$. In this case, the velocity $x \mapsto a(\partial_x S)$ does not satisfy the one-sided Lipschitz estimate (8). Therefore we cannot define measure

solutions in the sense of duality. However, we can prove, using the arguments in e.g. [8] that if $\rho^{ini} \in L^1 \cap W^{1,\infty}(\mathbb{R})$, we have global in time existence of solutions in $L^1 \cap W^{1,\infty}(\mathbb{R})$.

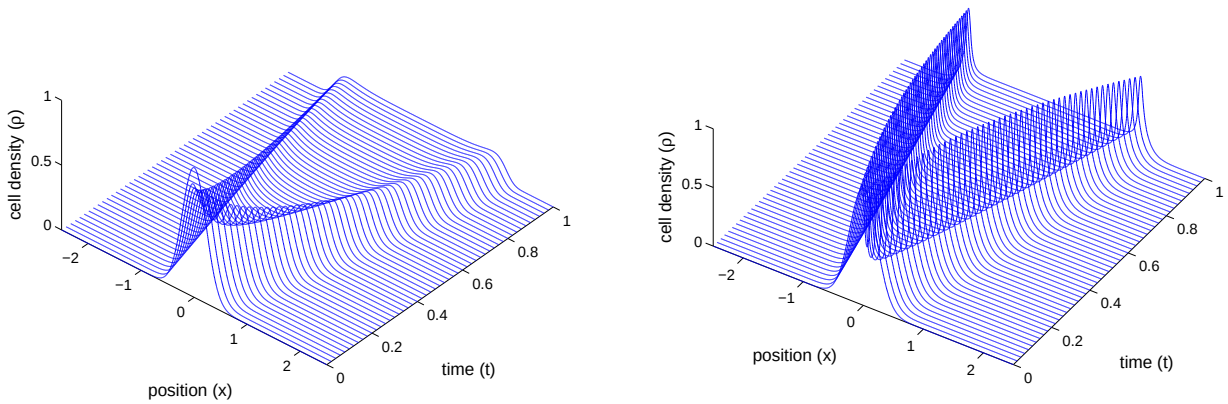

Figure 2: Dynamics of the cell density in the repulsive case, i.e. for a non-increasing function $a(x) = -2/\pi$ Atan(kx). Left : $k = 10$; Right : $k = 50$.

We observe in Figure 2 that support of the solution increases in time. It corresponds to the fact that cells repulse themselves. The particle scheme proposed in [7] does not allow to get satisfying numerical results in the repulsive case. In fact in this latter scheme, we approximate the solution by a finite sum of Dirac masses. However, as we noticed above, duality solutions can not be defined in this case. Therefore we do not know how to solve the system for an initial data given by a sum of Dirac masses.

Finally, Figure 3 displays the dynamic of cells density in the repulsive case $a(x) = -2/\pi$ Atan$(10x)$ and for the initial data $\rho^{ini}(x) = e^{-10(x-0.7)^2} + e^{-10(x+0.7)^2}$.

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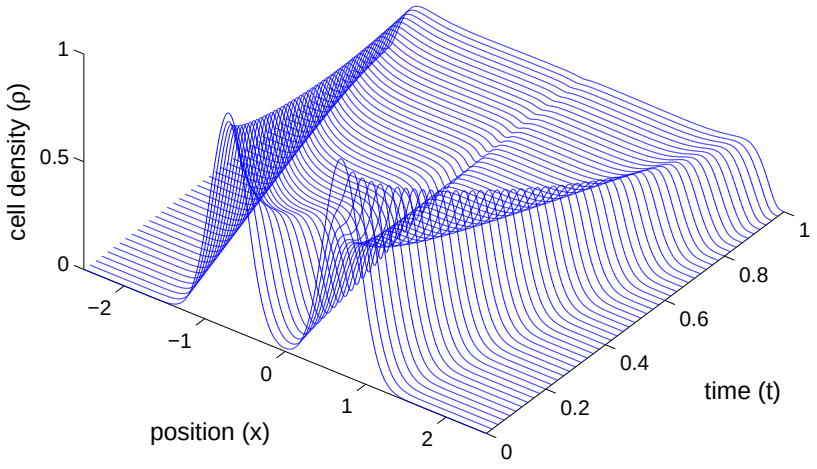

Figure 3: Dynamics of the cell density for an initial data given by a sum of 2 regular bumps in the repulsive case for $a(x) = -2/\pi$ Atan$(10x)$.